

## Author index to volume 254

- Adamo, C., R. Telesca and F. Lelj, On the nature of the cobalt–nitrogen bond in the  $\text{CoN}_2^+$  complex. A theoretical study 254 (1996) 314
- Adamson, R.D., J.P. Dombroski and P.M.W. Gill, Chemistry without Coulomb tails 254 (1996) 329
- Andrews, L., see Brabson, G.D. 254 (1996) 94
- Aoiz, F.J., L. Bañares, V.J. Herrero, K. Stark and H.-J. Werner, Reaction cross sections and rate constants for the  $\text{F} + \text{H}_2(\text{D}_2) \rightarrow \text{HF}(\text{DF}) + \text{H}(\text{D})$  reactions from quasiclassical trajectory calculations on a potential energy surface 254 (1996) 341
- Aucar, G.A., Restrictions on ground state average values imposed by time reversal symmetry 254 (1996) 13
- Aurentz, D.J., see Mueller, K.T. 254 (1996) 281
- Balasubramanian, K., see Roszak, S. 254 (1996) 274
- Ballard, C.C., M. Hada, H. Kaneko and H. Nakatsuji, Relativistic study of nuclear magnetic shielding constants: hydrogen halides 254 (1996) 170
- Bañares, L., see Aoiz, F.J. 254 (1996) 341
- Banhart, F., see Füller, T. 254 (1996) 372
- BelBruno, J.J., Ab initio calculations of the energies of the ring-opened and ring-closed isomers of  $\text{C}_2\text{H}_4\text{S}^{++}$  254 (1996) 321
- Bhatti, Z.A., see Green, N.J.B. 254 (1996) 358
- Bloemink, H.I., J.H. Holloway and A.C. Legon, Mulliken inner complexes  $[(\text{CH}_3)_3\text{NCl}]^+ \cdots \text{F}^-$  in pre-reactive mixtures of trimethylamine and chlorine monofluoride: identification and characterisation by rotational spectroscopy 254 (1996) 59
- Bosanac, S.D. and J.N. Murrell, Collision dynamics for small helium cluster ions 254 (1996) 69
- Bourbon, C., M. Brioukov, B. Hanoune, J.P. Sawersyn and P. Devolder, Flow tube/LIF measurements of the rate constants for the reactions with NO of  $\text{CF}_3\text{O}$  and  $\text{CF}_3\text{O}_2$  radicals 254 (1996) 203
- Boutchard, C., see Riley, M.J. 254 (1996) 403
- Brabson, G.D., J.C. Dillon and L. Andrews, Infrared spectrum of SeF in solid argon 254 (1996) 94
- Brioukov, M., see Bourbon, C. 254 (1996) 203
- Brown, N.J., see Chang, J. 254 (1996) 147
- Brugè, F., S.L. Fornili, G.G. Malenkov, M.B. Palma-Vittorelli and M.U. Palma, Solvent-induced forces on a molecular scale: non-additivity, modulation and causal relation to hydration 254 (1996) 283
- Byszewski, P., see Świetlik, R. 254 (1996) 73

- Cahill, P.A., Ab initio computational study of selected  $C_{60}H_6$  isomers 254 (1996) 257
- Campargue, A., see Romanini, D. 254 (1996) 52
- Chang, J. and N.J. Brown, Sensitivity of the product vibrational distribution of the  $F + H_2$  reaction to the T5A potential energy surface 254 (1996) 147
- Chapovsky, P.L., Nuclear spin conversion in  $CH_3F$  induced by magnetic particles 254 (1996) 1
- Chen, X., see Zhao, J. 254 (1996) 21
- Chernook, A.V., U. Rempel, C. von Borczyskowski, A.M. Shulga and E.I. Zenkevich, Formation and optical properties of self-organized pentameric porphyrin arrays 254 (1996) 229
- Cho, K., see Lee, S. 254 (1996) 128
- Corongiu, G., see Martorana, V. 254 (1996) 292
- Cory, D.G., see Maas, W.E. 254 (1996) 165
- Davidovich, R.L., see Gabuda, S.P. 254 (1996) 89
- Devolder, P., see Bourbon, C. 254 (1996) 203
- De Yong, L.V., see Smit, K.J. 254 (1996) 197
- Dhindsa, A.S., see Wenseleers, W. 254 (1996) 410
- Dillon, J.C., see Brabson, G.D. 254 (1996) 94
- Dombroski, J.P., see Adamson, R.D. 254 (1996) 329
- Drexhage, K.H., see Sauer, M. 254 (1996) 223
- Dubost, H., see Kolos, R. 254 (1996) 47
- Eletskii, A.V., see Vorob'ev, V.S. 254 (1996) 263
- Elking, M.D., see He, G. 254 (1996) 184
- Endo, Y., see Kohguchi, H. 254 (1996) 397
- Epifanov, S.Yu.,  $L^2$  golden rule-RRG combined method for resonance energies and widths 254 (1996) 141
- Era, M., see Hattori, T. 254 (1996) 103
- Eriksson, L.A., see Nguyen, M.T. 254 (1996) 307
- Ernst, R.R., see Gan, Z. 254 (1996) 349
- Fornili, S.L., see Brugè, F. 254 (1996) 283
- Füller, T. and F. Banhart, In situ observation of the formation and stability of single fullerene molecules under electron irradiation 254 (1996) 372
- Gabuda, S.P., S.G. Kozlova and R.L. Davidovich, Unexpected chemical bonding in quantum confined layers in  $TiZrF_5$  254 (1996) 89
- Gan, Z., D.M. Grant and R.R. Ernst, NMR chemical shift anisotropy measurements by RF driven rotary resonance 254 (1996) 349
- Gehret, O. and M.P. Irion, Reactions of  $Fe_n^+$  clusters ( $n = 2-11$ ) with  $C_6H_6$  and  $C_6D_6$ . Ligand isomerization in the benzene precursor ion  $Fe_4(C_2H_2)_3^+$  254 (1996) 379
- Geiger, F. and G. Marowsky, Optical second-harmonic generation from oligothiophene films 254 (1996) 179
- Gilch, P., M. Linsenmann, W. Haas and U.E. Steiner, Magnetic field effect on the photooxidation efficiency of ferrocene 254 (1996) 384
- Gill, P.M.W., see Adamson, R.D. 254 (1996) 329
- Goovaerts, E., see Wenseleers, W. 254 (1996) 410
- Grant, D.M., see Gan, Z. 254 (1996) 349
- Gray, R., see Smit, K.J. 254 (1996) 197
- Green, N.J.B. and Z.A. Bhatti, Steady-state approximation to the master equation for thermal dissociation reactions 254 (1996) 358

- Haas, W., see Gilch, P. 254 (1996) 384
- Haas, Y., see Zingher, E. 254 (1996) 213
- Hada, M., see Ballard, C.C. 254 (1996) 170
- Hanazaki, I., see Tanaka, N. 254 (1996) 40
- Hanoun, B., see Bourbon, C. 254 (1996) 203
- Hashimoto, H., see Mori, Y. 254 (1996) 84
- Hattori, T., T. Taira, M. Era, T. Tsutsui and S. Saito, Highly efficient electroluminescence from a heterostructure device combined with emissive layered-perovskite and an electron-transporting organic compound 254 (1996) 103
- He, G., M.D. Elking and Z. Xu, Observation of electrochemical reduction in the electrical double layer region using sum frequency generation spectroscopy 254 (1996) 184
- Herrero, V.J., see Aoiz, F.J. 254 (1996) 341
- Hinnen, P.C. and W. Ubachs, Further tests concerning the hypothesis of  $H_2$  as the carrier of diffuse interstellar bands 254 (1996) 32
- Hitchman, M.A., see Riley, M.J. 254 (1996) 403
- Holloway, J.H., see Bloemink, H.I. 254 (1996) 59
- Houzouji, T., N. Saito, A. Kudo and T. Sakata, Electroluminescence of  $TiO_2$  film and  $TiO_2:Cu^{2+}$  film prepared by the sol-gel method 254 (1996) 109
- Huang, Y. and M. Sulkes, Anomalous short fluorescence lifetimes in jet cooled 4-hydroxyindole. Evidence for excited state tautomerism and proton transfer in clusters 254 (1996) 242
- Irion, M.P., see Gehret, O. 254 (1996) 379
- Jackson, K. and B. Nellerme,  $Zr@Si_{20}$ : a strongly bound Si endohedral system 254 (1996) 249
- Jarvie, T.P., see Mueller, K.T. 254 (1996) 281
- Joannopoulos, J.D., see Lee, S. 254 (1996) 128
- Kaneko, H., see Ballard, C.C. 254 (1996) 170
- Kang, H.C., A computational study of the structures of Van der Waals and hydrogen-bonded complexes of ethene and ethyne 254 (1996) 135
- Kawasaki, M. and H. Uchiki, Formation of silver halide monolayer on Au-covered  $Ag(111)$  in alkali halide solution 254 (1996) 98
- Kendler, S., see Zingher, E. 254 (1996) 213
- Kierzkowski, P., B. Pranszke and A. Kowalski, Electronic branching ratios in the chemiluminescent reactions of  $Sr(^1S)$  and  $Sr(^3P, ^1D)$  atoms with  $ICl$  and  $IBr$  254 (1996) 391
- Kim, J., see Lee, S. 254 (1996) 128
- Kim, K.S., see Lee, S. 254 (1996) 128
- Kohguchi, H., Y. Ohshima and Y. Endo, Laser-induced fluorescence spectra and the observation of quantum beats in the  $\tilde{A}^2\Pi_1-\tilde{X}^2\Pi_1$  transition of the HCCS radical 254 (1996) 397
- Kolos, R., A. Salloum and H. Dubost, Molecular hydrogen isotopomers as traps of vibrational energy in low temperature matrices 254 (1996) 47
- Kowalska, E., see Świątek, R. 254 (1996) 73
- Kowalski, A., see Kierzkowski, P. 254 (1996) 391
- Kozlova, S.G., see Gabuda, S.P. 254 (1996) 89
- Krausz, E.R., see Riley, M.J. 254 (1996) 403
- Kudo, A., see Houzouji, T. 254 (1996) 109
- Kulkarni, S.A., Electron correlation effects on the topography of molecular electrostatic potentials 254 (1996) 268
- Kuprievich, V.A., Unified coupling operator for 'non-Roothaan' open-shell states of high-symmetry molecules 254 (1996) 365

- Lee, J.Y., see Lee, S. 254 (1996) 128
- Lee, S., S.J. Lee, J.Y. Lee, J. Kim, K.S. Kim, I. Park, K. Cho and J.D. Joannopoulos, Ab initio study of water hexamer anions 254 (1996) 128
- Lee, S.J., see Lee, S. 254 (1996) 128
- Legon, A.C., see Bloemink, H.I. 254 (1996) 59
- Lelj, F., see Adamo, C. 254 (1996) 314
- Levin, E., see Stallcop, J.R. 254 (1996) 25
- Lin, S.H., see Tang, J. 254 (1996) 6
- Linsenmann, M., see Gilch, P. 254 (1996) 384
- Liu, W.-K., see Wang, Y.-N. 254 (1996) 122
- Maas, W.E. and D.G. Cory, Discrete magnetization gratings in NMR spectroscopy 254 (1996) 165
- Malenkov, G.G., see Brugè, F. 254 (1996) 283
- Marowsky, G., see Geiger, F. 254 (1996) 179
- Martorana, V., G. Corongiu and M.U. Palma, Correlated solvent-induced forces on a protein at single residue resolution: relation to conformation, stability, dynamics and function 254 (1996) 292
- Mori, Y., K. Yamano and H. Hashimoto, Bistable aggregate of all-trans-astaxanthin in an aqueous solution 254 (1996) 84
- Mueller, K.T., T.P. Jarvie, D.J. Aurentz and B.W. Roberts, Erratum and Comment on "The REDOR transform: direct calculation of internuclear couplings from dipolar-dephasing NMR data" (Chem. Phys. Letters 242 (1996) 535-542) 254 (1996) 281
- Murrell, J.N., see Bosanac, S.D. 254 (1996) 69
- Nakano, M., see Yamada, S. 254 (1996) 158
- Nakatsuji, H., see Ballard, C.C. 254 (1996) 170
- Nellermoe, B., see Jackson, K. 254 (1996) 249
- Nguyen, M.T., A. Van Keer, L.A. Eriksson and L.G. Vanquickenborne, Some calculated properties of phenylphosphinidene ( $C_6H_5P$ ) 254 (1996) 307
- Ohshima, Y., see Kohguchi, H. 254 (1996) 397
- Okada, K., M. Yamaji and H. Shizuka, Laser flash photolysis studies on the induced-quenching process competing with hydrogen atom abstraction of triplet benzophenone. Heavy atom effect 254 (1996) 79
- Palma, M.U., see Brugè, F. 254 (1996) 283
- Palma, M.U., see Martorana, V. 254 (1996) 292
- Palma-Vittorelli, M.B., see Brugè, F. 254 (1996) 283
- Park, I., see Lee, S. 254 (1996) 128
- Partridge, H., see Stallcop, J.R. 254 (1996) 25
- Persson, B.N.J., Theory of friction: on the origin of the stick-slip motion of lubricated surfaces 254 (1996) 114
- Pranszke, B., see Kierzkowski, P. 254 (1996) 391
- Rempel, U., see Chernook, A.V. 254 (1996) 229
- Riley, M.J., C. Boutchard, E.R. Krausz and M.A. Hitchman, Observation of a magnetic dipole origin in the spectrum of the square planar  $CuCl_4^{2-}$  ion 254 (1996) 403
- Roberts, B.W., see Mueller, K.T. 254 (1996) 281

- Romanini, D. and A. Campargue, Vibrational overtone spectroscopy of the  $4_1$  band of  $\text{CHF}_3$  254 (1996) 52
- Rozsak, S. and K. Balasubramanian, Electronic structure and thermodynamic properties of  $\text{YIrC}$  and  $\text{YIrC}_2$  254 (1996) 274
- Saito, N., see Houzouji, T. 254 (1996) 109
- Saito, S., see Hattori, T. 254 (1996) 103
- Sakata, T., see Houzouji, T. 254 (1996) 109
- Salloum, A., see Kolos, R. 254 (1996) 47
- Sauer, M., K.H. Drexhage, C. Zander and J. Wolfrum, Diode laser based detection of single molecules in solutions 254 (1996) 223
- Sawerysyn, J.P., see Bourbon, C. 254 (1996) 203
- Schulz, W.W., Note on the computation of the multipole tensor in spherical harmonics 254 (1996) 337
- Shigemoto, I., see Yamada, S. 254 (1996) 158
- Shizuka, H., see Okada, K. 254 (1996) 79
- Shulga, A.M., see Chernook, A.V. 254 (1996) 229
- Smit, K.J., L.V. De Yong and R. Gray, Observation of infrared emission spectra from silicon combustion products 254 (1996) 197
- So, S.P., A Gaussian-2 molecular orbital study of the sigmatropic 1,3-hydrogen shift in 1-silapropene 254 (1996) 302
- Stallcop, J.R., H. Partridge and E. Levin,  $\text{H}-\text{H}_2$  collision integrals and transport coefficients 254 (1996) 25
- Stark, K., see Aoiz, F.J. 254 (1996) 341
- Steiner, J.E., see Gilch, P. 254 (1996) 384
- Sulkes, M., see Huang, Y. 254 (1996) 242
- Świetlik, R., P. Byszewski and E. Kowalska, Interactions of  $\text{C}_{60}$  with organic molecules in solvate crystals studied by infrared spectroscopy 254 (1996) 73
- Taira, T., see Hattori, T. 254 (1996) 103
- Takayanagi, M., see Tanaka, N. 254 (1996) 40
- Tanaka, N., M. Takayanagi and I. Hanazaki, Nascent rotational and vibrational distributions in  $^{16}\text{OH}$  and  $^{18}\text{OH}$  produced in the reaction of  $\text{O}(^1\text{D})$  with  $\text{H}_2^{18}\text{O}$  254 (1996) 40
- Tang, J. and S.H. Lin, Oscillations and non-exponential decays in electron-transfer reactions 254 (1996) 6
- Telesca, R., see Adamo, C. 254 (1996) 314
- Tsutsui, T., see Hattori, T. 254 (1996) 103
- Ubachs, W., see Hinnen, P.C. 254 (1996) 32
- Uchiki, H., see Kawasaki, M. 254 (1996) 98
- Underhill, A.E., see Wenseleers, W. 254 (1996) 410
- Van Keer, A., see Nguyen, M.T. 254 (1996) 307
- Vanquickenborne, L.G., see Nguyen, M.T. 254 (1996) 307
- Von Borczyskowski, C., see Chernook, A.V. 254 (1996) 229
- Vorob'ev, V.S. and A.V. Eletskii, Similarity laws and thermodynamic quantities for fullerite  $\text{C}_{60}$  254 (1996) 263

- Wang, G., see Zhao, J. 254 (1996) 21
- Wang, Y.-N. and W.-K. Liu, Wake potential of an ion moving slowly near a solid surface 254 (1996) 122
- Wenseleers, W., E. Goovaerts, A.S. Dhindsa and A.E. Underhill, Third order nonlinear optical polarisability induced by real electronic excitations in transition metal diimine and dithiolene complexes 254 (1996) 410
- Werner, H.-J., see Aoiz, F.J. 254 (1996) 341
- Wolfrum, J., see Sauer, M. 254 (1996) 223
- Xu, Z., see He, G. 254 (1996) 184
- Yamada, S., M. Nakano, I. Shigemoto and K. Yamaguchi, Static second hyperpolarizabilities  $\gamma$  of nitroxide radical and formaldehyde: evaluation of spatial contributions to  $\gamma$  by a hyperpolarizability density analysis 254 (1996) 158
- Yamaguchi, K., see Yamada, S. 254 (1996) 158
- Yamaji, M., see Okada, K. 254 (1996) 79
- Yamano, K., see Mori, Y. 254 (1996) 84
- Yoneyama, M., Optical modification of wave dynamics in a surface layer of the Mn-catalyzed Belousov-Zhabotinsky reaction 254 (1996) 191
- Zander, C., see Sauer, M. 254 (1996) 223
- Zenkevich, E.I., see Chernook, A.V. 254 (1996) 229
- Zhao, J., X. Chen and G. Wang, An analytic relationship between size and ionization potential of transition-metal clusters 254 (1996) 21
- Zingher, E., S. Kendler and Y. Haas, The photophysics of a photoreactive system in a supersonic jet. Styrene-trimethylamine 254 (1996) 213



